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From: Jan Delaval
Location: Biotech-Chem Library
Rem 1A51
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jan.delaval@uspto.gov

Search Notes

FILE 'USPATFULL' ENTERED AT 17:00:29 ON 23 JUN 2004
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FILE 'HCAPLUS' ENTERED AT 17:00:29 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE 'HCAOLD' ENTERED AT 17:00:29 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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=> s l3 and (?glaucom? or ocular? or intra(2a)ocular? or ophthal? or eye or intraocular?)
L4 5 L3 AND (?GLAUCOM? OR OCULAR? OR INTRA(2A) OCULAR? OR OPHTHAL? OR EYE OR INTRAOCULAR?)

=> dup rem l5
L5 IS NOT VALID HERE
The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> dup rem l4
DUPLICATE IS NOT AVAILABLE IN 'HCAOLD'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
PROCESSING COMPLETED FOR L4
L5 5 DUP REM L4 (0 DUPLICATES REMOVED)

=> d l5 abs ibib kwic hitstr 1-5

L5 ANSWER 1 OF 5 USPATFULL on STN
AB Provided is a method of treating or ameliorating certain fibrotic diseases or other indications in an animal, including a human, comprising administering an effective amount of a compound of the formula I:

Y--Ar.sup..sym..X.sup.-

wherein Ar.sup..sym. is heteroaryl with a quaternary nitrogen, Y defines certain substitutions on the quaternary nitrogen, and X.sup.- is anion.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER:	2004:127511 USPATFULL		
TITLE:	Method for treating fibrotic diseases or other indications IIIC		
INVENTOR(S):	Wagle, Dilip, New York, NY, UNITED STATES Gall, Martin, Morristown, NJ, UNITED STATES Bell, Stanley C., Narberth, PA, UNITED STATES LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES		
	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004097495	A1	20040520

APPLICATION INFO.: US 2003-691839 A1 20031023 (10)
RELATED APPLN. INFO.: Continuation of Ser. No. US 2001-36857, filed on 31 Dec 2001, PENDING

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-259294P	20001229 (60)
	US 2001-259238P	20010102 (60)
	US 2001-296246P	20010606 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MINTZ, LEVIN, COHN, FERRIS, GLOVSKY, AND POPEO, P.C., ONE FINANCIAL CENTER, BOSTON, MA, 02111
NUMBER OF CLAIMS: 49
EXEMPLARY CLAIM: 1
LINE COUNT: 3287
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM [0106] The effect of diabetes on the **eye** is called diabetic retinopathy and involves changes to the circulatory system of the retina. The earliest phase of the disease. . . . phases of the disease, continued abnormal vessel growth and scar tissue may cause serious problems such as retinal detachment and **glaucoma**. First agents are used to treat, prevent, reduce or ameliorate diabetic retinopathy. The agents can be administered by the methods described below, including by topical administration to the **eye**. The agents can also be administered by intravitreal implant.

SUMM [0123] Pharmaceutical compositions of the invention include administering an **intraocular** pressure decreasing amount of a compound of the formula I.

SUMM [0325] Compositions can also be used to deliver the compound to the site where activity is desired; such as **eye** drops, gels and creams for **ocular** disorders.

SUMM . . . compositions of this invention include aqueous solutions comprising a safe and effective amount of a subject compound intended for topical **intraocular** administration. Such compositions preferably comprise from about 0.01% to about 0.8% w/v of a subject compound, more preferably from about. . .

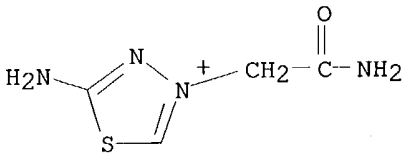
SUMM [0330] The compounds of the invention are administered by **ocular**, oral, parenteral, including, for example, using formulations suitable as **eye** drops. For **ocular** administration, ointments or droppable liquids may be delivered by **ocular** delivery systems known to the art such as applicators or **eye** droppers. Such compositions can include mucomimetics such as hyaluronic acid, chondroitin sulfate, hydroxypropyl methylcellulose or polyvinyl alcohol, preservatives such as. . .

IT 13076-43-2P 63828-55-7P **454704-85-9P 454704-86-0P 454704-87-1P** 454704-88-2P 454704-89-3P 454704-90-6P 454704-91-7P
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT **454704-85-9P 454704-86-0P 454704-87-1P**
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 454704-85-9 USPATFULL

CN 1,3,4-Thiadiazolium, 5-amino-3-(2-amino-2-oxoethyl)-, bromide (9CI) (CA INDEX NAME)



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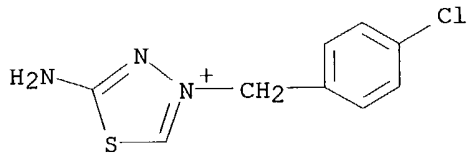
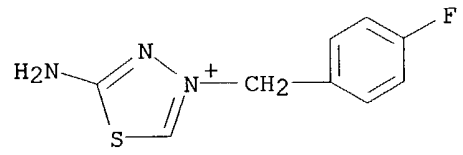
RN 454704-86-0 USPATFULL
CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

RN 454704-87-1 USPATFULL
CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-fluorophenyl)methyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

L5 ANSWER 2 OF 5 USPATFULL on STN
AB Provided, among things, is a method of treating or ameliorating an indication of the invention in an animal, including a human, comprising administering an effective amount of a compound of formula I: ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
ACCESSION NUMBER: 2003:4153 USPATFULL
TITLE: Method for treating fibrotic diseases or other indications VI

INVENTOR(S): Gall, Martin, Morristown, NJ, UNITED STATES
PATENT ASSIGNEE(S): Alteon, Inc., Ramsey, NJ, UNITED STATES (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003004194	A1	20030102	
	US 6596745	B2	20030722	
APPLICATION INFO.:	US 2002-158344	A1	20020530	(10)

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2001-294438P	20010530	(60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: ALLEN BLOOM, C/O DECHERT, PRINCETON PIKE CORPORATION CENTER, P.O. BOX 5218, PRINCETON, NJ, 08543-5218
NUMBER OF CLAIMS: 23
EXEMPLARY CLAIM: 1
LINE COUNT: 1243
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

DETD [0068] The effect of diabetes on the **eye** is called diabetic retinopathy and involves changes to the circulatory system of the retina. The earliest phase of the disease. . . ameliorate diabetic retinopathy. The fisrt agents can be administered by the methods described below, including by topical administration to the **eye** . The agents can also be administered by intravitreal implant.

DETD [0114] Compositions can also be used to deliver the compound to the site where activity is desired; such as **eye** drops, gels and creams for **ocular** disorders.

DETD . . . compositions of this invention include aqueous solutions comprising a safe and effective amount of a subject compound intended for topical **intraocular** administration. Such compositions preferably comprise from about 0.01% to about 0.8% w/v of a subject compound, more preferably from about. . .

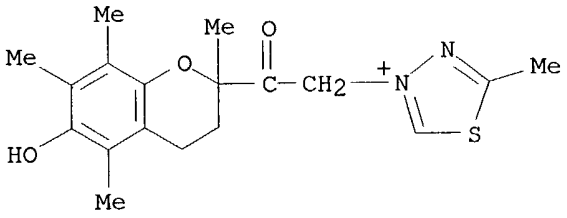
DETD [0119] The compounds of the invention are administered by **ocular** , oral, parenteral, including, for example, using formulations suitable as **eye** drops. For **ocular** administration, ointments or droppable liquids may be delivered by **ocular** delivery systems known to the art such as applicators or **eye** droppers. Such compositions can include mucomimetics such as hyaluronic acid, chondroitin sulfate, hydroxypropyl methylcellulose or polyvinyl alcohol, preservatives such as. . .

IT 477252-66-7P 477252-67-8P 477252-68-9P 477252-69-0P
477252-70-3P 477252-71-4P 477252-72-5P
477252-73-6P 477252-74-7P 477252-75-8P 477252-76-9P
477252-77-0P 477252-78-1P 477252-79-2P 477252-80-5P
477252-81-6P 477252-82-7P 477252-83-8P
477252-84-9P 477252-85-0P 477252-86-1P 477252-87-2DP, derivs.
(method for treating fibrotic diseases or other indications)

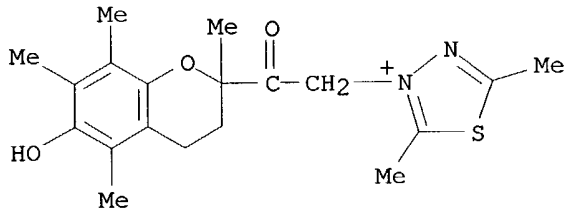
IT **477252-70-3P 477252-71-4P 477252-72-5P**
477252-73-6P 477252-81-6P 477252-82-7P
477252-83-8P 477252-84-9P
(method for treating fibrotic diseases or other indications)

RN 477252-70-3 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-

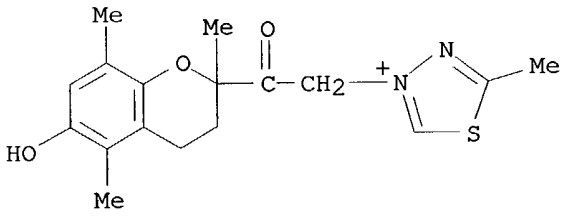
benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



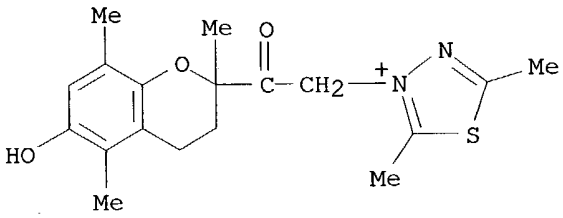
RN 477252-71-4 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



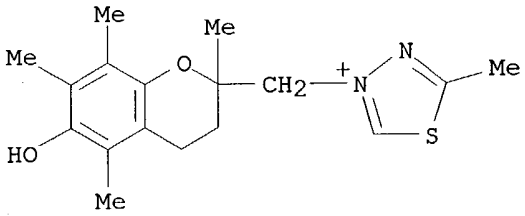
RN 477252-72-5 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



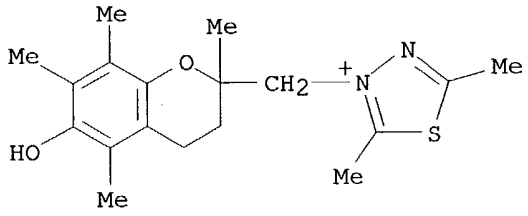
RN 477252-73-6 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



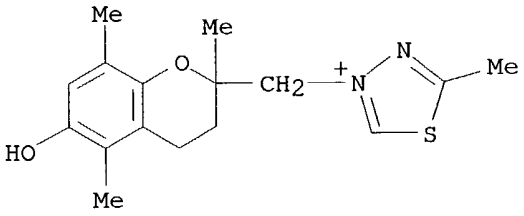
RN 477252-81-6 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



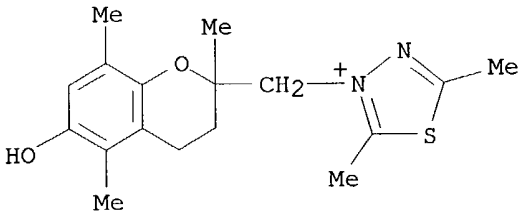
RN 477252-82-7 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



RN 477252-83-8 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 477252-84-9 USPATFULL
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 5 USPATFULL on STN

AB Provided is a method of treating or ameliorating certain fibrotic diseases or other indications in an animal, including a human, comprising administering an effective amount of a compound of the formula I:

Y--Ar.sym..multidot.X.sup.--

wherein:

a. Ar is a five or six membered heteroaryl ring having a first ring nitrogen and optionally second or third ring nitrogens, with the remaining ring atoms being carbon, oxygen, or sulfur, provided the first nitrogen of Ar is a quaternary nitrogen and Ar is not thiazolium, oxazolium or imidazolium;

b. Y is substituted on the first ring nitrogen, with the proviso that if Ar is pyrazole, indazole, (1,2,3)-triazole, benzotriazole, or (1,2,4)-triazole, the second ring nitrogen is substituted

C. Y is:

1. a group of the formula --CH(R.sup.5)--R.sup.6 [as preferred in one embodiment]

(a) wherein R.sup.5 is hydrogen, alkyl, cycloalkyl-, alkenyl-, alkynyl-, aminoalkyl-, hydroxy[C.sub.1 to C.sub.6]alkyl, dialkylaminoalkyl-, (N-[C.sub.6 or C.sub.10]aryl)(N-alkyl)aminoalkyl-, piperidin-1-ylalkyl-, pyrrolidin-1-ylalkyl, azetidinylalkyl, 4-alkylpiperazin-1-ylalkyl, 4-alkylpiperidin-1-ylalkyl, 4-[C.sub.6 or C.sub.10]arylpiperazin-1-ylalkyl, 4-[C.sub.6 or C.sub.10]arylpiperidin-1-ylalkyl, azetidin-1-ylalkyl, morpholin-4-ylallcyl, thiomorpholin-4-ylalkyl, piperazin-1-ylalkyl, piperidin-1-ylalkyl, [C.sub.6 or C.sub.10]aryl, or independently the same as R.sup.6;

(b) wherein R.sup.6 is

(1) hydrogen, alkyl (which may be substituted by alkoxycarbonyl)-, alkenyl, alkynyl, cyano-, cyanoalkyl-, or Rs, wherein Rs is a [C.sub.6 or C.sub.10]aryl or a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms selected from the group consisting of oxygen, nitrogen and sulfur; or

(2) a group of the formula --W--R.sup.7 [as preferred in one embodiment], wherein R.sup.7 is alkyl, alkoxy, hydroxy, or Rs [as preferred in one embodiment], wherein W is --C(.dbd.O)-- or

--S(O).sub.2--;

(3) a group of the formula --W--OR.sup.8 wherein R.sup.8 is hydrogen or alkyl,

(4) a group of the formula --CH(OH)Rs; or

(5) a group of the formula --W--N(R.sup.9)R.sup.10, wherein

(a) R.sup.9 is hydrogen and R.sup.10 is an alkyl or cycloalkyl, optionally substituted; or

(b) R.sup.9 is hydrogen or alkyl and R.sup.10 is Ar; or

(c) R.sup.9 is hydrogen or alkyl, R.sup.10 is a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms are selected from the group consisting of oxygen, nitrogen and sulfur; or

(d) R.sup.9 and R.sup.10 are both alkyl groups; or

(e) R.sup.9 and R.sup.10 together with N form a heterocycle containing 4-10 ring atoms which can incorporate up to one additional heteroatom selected from the group of N, O or S in the ring, wherein the heterocycle is optionally substituted; or

(f) R.sup.9 and R.sup.10 are both hydrogen; or

2. --NH.sub.2, and

e. X is a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt, or

(B) a pharmaceutically acceptable salt of the compound.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2002:323196 USPATFULL
TITLE: Method for treating fibrotic diseases or other indications IIIC

INVENTOR(S): Wagle, Dilip, New York, NY, UNITED STATES
Gall, Martin, Morristown, NJ, UNITED STATES
Bell, Stanley C., Narberth, PA, UNITED STATES
LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002183365	A1	20021205	
APPLICATION INFO.:	US 2001-36857	A1	20011231	(10)

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2001-296246P	20010606	(60)
	US 2001-259238P	20010102	(60)
	US 2000-259294P	20001229	(60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: ALLEN BLOOM, C/O DECHERT, PRINCETON PIKE CORPORATION

CENTER, P.O. BOX 5218, PRINCETON, NJ, 08543-5218
NUMBER OF CLAIMS: 49
EXEMPLARY CLAIM: 1
LINE COUNT: 3334
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM [0105] The effect of diabetes on the **eye** is called diabetic retinopathy and involves changes to the circulatory system of the retina. The earliest phase of the disease. . . phases of the disease, continued abnormal vessel growth and scar tissue may cause serious problems such as retinal detachment and **glaucoma**. First agents are used to treat, prevent, reduce or ameliorate diabetic retinopathy. The agents can be administered by the methods described below, including by topical administration to the **eye**. The agents can also be administered by intravitreal implant.

SUMM [0122] Pharmaceutical compositions of the invention include administering an **intraocular** pressure decreasing amount of a compound of the formula I.

SUMM [0320] Compositions can also be used to deliver the compound to the site where activity is desired; such as **eye** drops, gels and creams for **ocular** disorders.

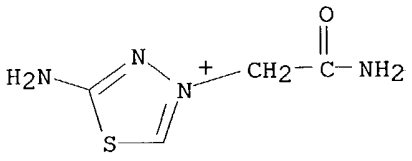
SUMM . . . compositions of this invention include aqueous solutions comprising a safe and effective amount of a subject compound intended for topical **intraocular** administration. Such compositions preferably comprise from about 0.01% to about 0.8% w/v of a subject compound, more preferably from about. . .

SUMM [0325] The compounds of the invention are administered by **ocular**, oral, parenteral, including, for example, using formulations suitable as **eye** drops. For **ocular** administration, ointments or droppable liquids may be delivered by **ocular** delivery systems known to the art such as applicators or **eye** droppers. Such compositions can include mucomimetics such as hyaluronic acid, chondroitin sulfate, hydroxypropyl methylcellulose or polyvinyl alcohol, preservatives such as. . .

IT 13076-43-2P 63828-55-7P **454704-85-9P 454704-86-0P** **454704-87-1P** 454704-88-2P 454704-89-3P 454704-90-6P 454704-91-7P
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

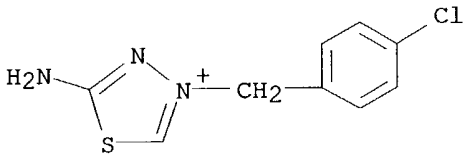
IT **454704-85-9P 454704-86-0P 454704-87-1P**
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 454704-85-9 USPATFULL
CN 1,3,4-Thiadiazolium, 5-amino-3-(2-amino-2-oxoethyl)-, bromide (9CI) (CA INDEX NAME)



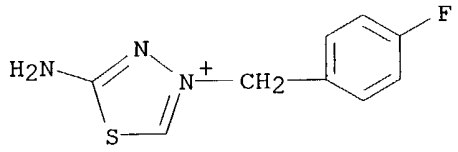
● Br^-

RN 454704-86-0 USPATFULL
CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



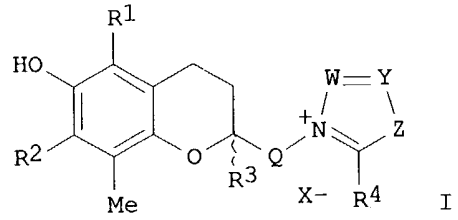
● Cl^-

RN 454704-87-1 USPATFULL
CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-fluorophenyl)methyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

L5 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
GI

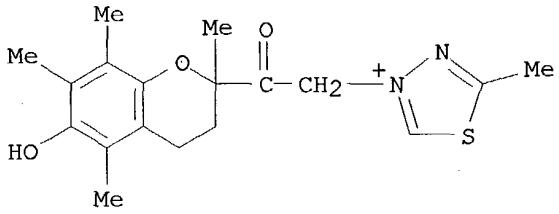


I

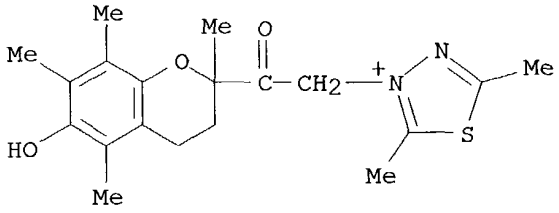
AB Provided, among things, is a method of treating or ameliorating an indication of the invention in an animal, including a human, comprising administering an effective amount of a compound of formula I, wherein: W and Y are independently N or, resp., CRW or CRY; Z is O, S or NRZ; Q is -CH2- or -(CO)-CH2-, where the methylne is bounded to a ring nitrogen; RW and RY are independently hydrogen, alkyl, -C.tplbond.CRE, -CH2-C.tplbond.CRP, aryl, alkylamino, arylamino, C(O)NH3, S(O)2NH2, etc.; RZ is alkyl,

(Uses)
(method for treating fibrotic diseases or other indications)

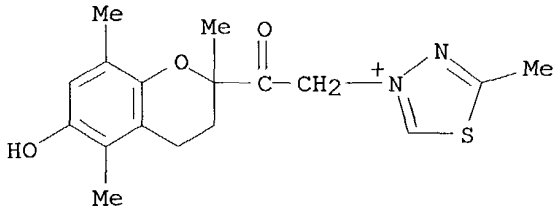
RN 477252-70-3 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



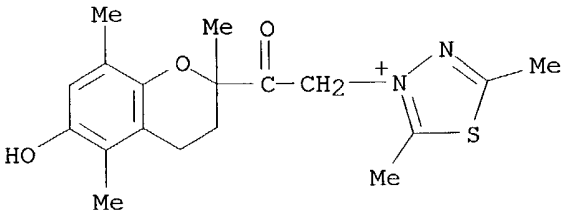
RN 477252-71-4 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



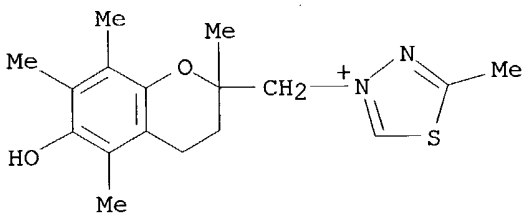
RN 477252-72-5 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



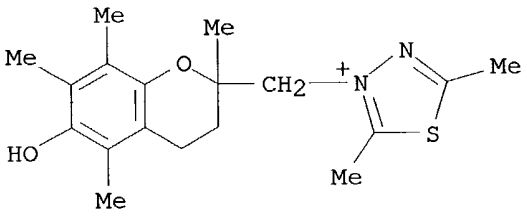
RN 477252-73-6 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



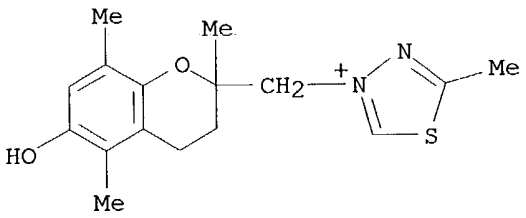
RN 477252-81-6 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 477252-82-7 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)

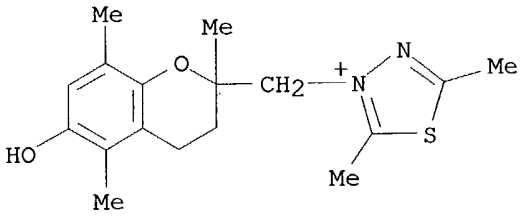


RN 477252-83-8 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)

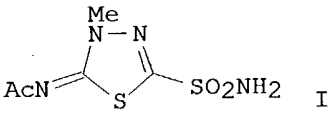


RN 477252-84-9 HCAPLUS
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-

benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB The relation between physicochem. properties and lowering of **intraocular** pressure (IOP) was studied in rabbits after topical application of a series of 5-acylimino- and related imino-substituted analogs of methazolamide (Compound 4) (I). All the compds. had a KI vs. carbonic anhydrase C of about 10-8M. The parent methazolamide (5-acetyl) did not lower IOP, in contrast to the 5-CF3 acetyl compound (Compound 28). The 5-propionyl compound (6) unexpectedly was 3 times more water soluble than methazolamide and had 10 times greater CHCl3-buffer partition. The in vivo transcorneal permeability constant was 6 times greater than methazolamide. One h after 1 drop of a 2% suspension of Compound 6, anterior aqueous concentration (in micromolar) was 69 (for methazolamide, 8), the posterior aqueous concentration was 19 and concentration in the ciliary processes was 17.
The IOP dropped 2.2 mm Hg and returned to normal in 4 h. Other compds. in the series showed varying degrees of activity, ranging from Compound 28, which elicited an IOP fall of 3.5 mm Hg, to Compound 7, (n-pentyryl), for which the fall was 1.3 mm Hg. Also studied are substitutions for CH3 on the ring N at position 4. There are multiple criteria for in vivo activity; a major factor is the balance between water and lipid solubility The methazolamide analogs are compared with benzothiazole-2-sulfonamides, another class under investigation as topical carbonic anhydrase inhibitors designed to treat **glaucoma**.

ACCESSION NUMBER: 1987:546815 HCAPLUS
DOCUMENT NUMBER: 107:146815
TITLE: **Ocular** pharmacology of methazolamide analogs: distribution in the **eye** and effects on pressure after topical application
AUTHOR(S): Maren, Thomas H.; Bar-Ilan, Amir; Caster, Kenneth C.; Katritzky, Alan R.
CORPORATE SOURCE: Coll. Med., Univ. Florida, Gainesville, FL, 32610, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics

(1987), 241(1), 56-63
CODEN: JPETAB; ISSN: 0022-3565
DOCUMENT TYPE: Journal
LANGUAGE: English

TI **Ocular** pharmacology of methazolamide analogs: distribution in the **eye** and effects on pressure after topical application

AB The relation between physicochem. properties and lowering of **intraocular** pressure (IOP) was studied in rabbits after topical application of a series of 5-acylimino- and related imino-substituted analogs of methazolamide. . . solubility The methazolamide analogs are compared with benzothiazole-2-sulfonamides, another class under investigation as topical carbonic anhydrase inhibitors designed to treat **glaucoma**.

ST methazolamide analog distribution **eye intraocular** pressure

IT **Eye**
(**intraocular** pressure of, methazolamide analogs effect on, distribution in)

IT Biological transport
(of methazolamide analogs, by **eye**, lipophilicity in relation to)

IT Lipophilicity
(of methazolamide analogs, distribution in **eye** in relation to)

IT Molecular structure-biological activity relationship
(**intraocular** pressure-reducing, of methazolamide analogs)

IT 554-57-4, Methazolamide
RL: BIOL (Biological study)
(physicochem. properties and **ocular** pharmacol. of)

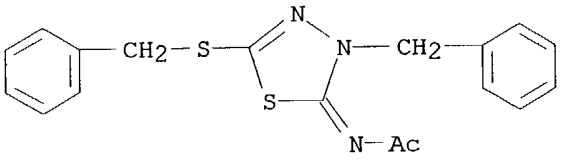
IT 64387-67-3P 105339-30-8P 109014-82-6P 109480-58-2P **109480-59-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to sulfonamide of)

IT 554-57-4DP, analogs 949-40-6P 952-59-0P 952-83-0P **965-11-7P** 1081-57-8P 55217-95-3P 81428-88-8P 81428-89-9P 93745-70-1P 93745-71-2P 109480-56-0P 109480-57-1P 109517-21-7P 109517-22-8P 110501-80-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and physicochem. properties and **ocular** pharmacol. of)

IT **109480-59-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to sulfonamide of)

RN 109480-59-3 HCAPLUS

CN Acetamide, N-[3-(phenylmethyl)-5-[(phenylmethyl)thio]-1,3,4-thiadiazol-2(3H)-ylidene]- (9CI) (CA INDEX NAME)

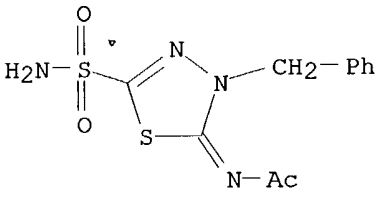


IT **965-11-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and physicochem. properties and **ocular** pharmacol. of)

RN 965-11-7 HCAPLUS

CN Acetamide, N-[5-(aminosulfonyl)-3-(phenylmethyl)-1,3,4-thiadiazol-2(3H)-ylidene]- (9CI) (CA INDEX NAME)



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provided by InfoChem.

STRUCTURE FILE UPDATES:   22 JUN 2004  HIGHEST RN 697737-72-7
DICTIONARY FILE UPDATES:  22 JUN 2004  HIGHEST RN 697737-72-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide can tot l51

L51  ANSWER 1 OF 3  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   459165-10-7  REGISTRY
CN   Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with
     trifluoromethanesulfonic acid (1:1) (9CI)  (CA INDEX NAME)
MF   C14 H15 N2 O2 . C F3 O3 S
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA  CAplus document type:  Patent
RL.P   Roles from patents:  PREP (Preparation); PRP (Properties)

     CM   1

     CRN  175979-55-2
     CMF  C14 H15 N2 O2
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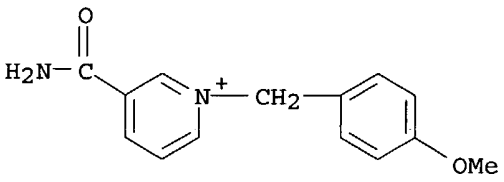


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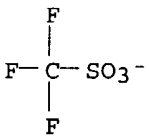
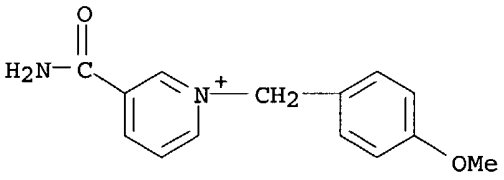


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:228603

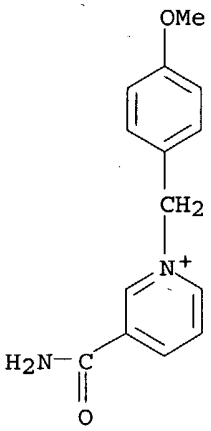
L51 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
RN **175979-55-2** REGISTRY
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H15 N2 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 124:316412

L51 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
RN 63828-55-7 REGISTRY
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-(p-methoxybenzyl)pyridinium chloride (7CI)
OTHER NAMES:
CN N-4'-Methoxybenzylnicotinamide chloride
MF C14 H15 N2 O2 . Cl
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent)
CRN (175979-55-2)



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8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:216955

REFERENCE 2: 125:300276

REFERENCE 3: 113:22794

REFERENCE 4: 108:166806

REFERENCE 5: 103:22428

REFERENCE 6: 99:104507

REFERENCE 7: 98:61940

REFERENCE 8: 87:80366

=> d his l51-

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L51 3 S L49,L50

FILE 'HCAOLD' ENTERED AT 16:09:07 ON 23 JUN 2004
L52 1 S L51
SEL AN
EDIT /AN /OREF

FILE 'HCAPLUS' ENTERED AT 16:09:38 ON 23 JUN 2004
L53 2 S E1
L54 1 S L53 NOT GRUDZINSKA ?/AU
L55 10 S L51

FILE 'USPATFULL, USPAT2' ENTERED AT 16:10:19 ON 23 JUN 2004
L56 4 S L51

FILE 'REGISTRY' ENTERED AT 16:10:53 ON 23 JUN 2004

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=> fil hcaold
FILE 'HCAOLD' ENTERED AT 16:11:07 ON 23 JUN 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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substance identification.  Title keywords, authors, patent
assignees, and patent information, e.g., patent numbers, are
now searchable from 1907-1966.  TIFF images of CA abstracts
printed between 1907-1966 are available in the PAGE
display formats.

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all substance data from the REGISTRY file.  Enter HELP FIRST for
more information.

=> d l52 all hitstr

L52  ANSWER 1 OF 1  HCAOLD  COPYRIGHT 2004 ACS on STN
AN   CA59:9970a  CAOLD
TI   action of base on quaternary salts of nicotinamide
AU   Dittmer, Donald C.; Kolyer, J. M.
IT    952-92-1   1652-58-0   1893-57-8   2996-08-9   4533-64-6   5096-13-9
     6621-73-4   6951-52-6  13502-54-0  19355-18-1  63828-55-7
     75340-29-3  92578-90-0  93807-08-0  93897-69-9  93946-35-1  94379-06-3
     95592-93-1  95592-94-2  95945-13-4  96003-72-4  96635-71-1  96650-48-5
     98310-77-1 100210-41-1 106141-61-1 106141-62-2 106141-68-8 106384-38-7
IT  63828-55-7
RN   63828-55-7  HCAOLD
CN   Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
     (CA INDEX NAME)
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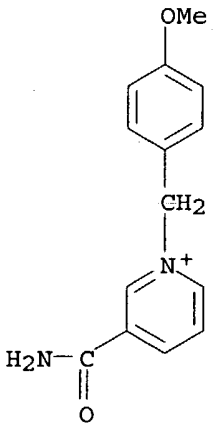

● Cl⁻

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 16:11:17 ON 23 JUN 2004
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FILE COVERS 1907 - 23 Jun 2004  VOL 140 ISS 26
FILE LAST UPDATED: 22 Jun 2004  (20040622/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l54 or l55
L57         11 L54 OR L55

=> d all hitstr tot

L57  ANSWER 1 OF 11  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:716518  HCAPLUS
DN   137:228603
ED   Entered STN:  20 Sep 2002
TI   NAD(P) mimic for use in enzymic redox reactions
IN   Fish, Richard H.; Kerr, John B.; Lo, Christine H.
PA   The Regents of the University of California, USA
SO   PCT Int. Appl., 63 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  C12Q
CC   7-3 (Enzymes)
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
PI   WO 2002072869     A2    20020919       WO 2002-US7444   20020311
     WO 2002072869     A3    20030227
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2003022266     A1    20030130       US 2001-805726   20010312
     US 6716596        B2    20040406
     EP 1373552        A2    20040102       EP 2002-725121   20020311
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRAI US 2001-805726    A     20010312
     WO 2002-US7444    W     20020311
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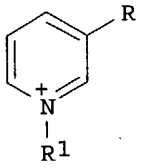
OS CASREACT 137:228603; MARPAT 137:228603

GI



I

AB Novel agents acting as co-factors for replacement of NAD(P)+/NAD(P)H co-enzyme systems in enzymic redox reactions are disclosed. A composition for replacement or regeneration of an NAD(P)+/NAD(P)H system in redox processes comprising (a) a polymer matrix, (b) a catalyst precursor, (3) a cofactor, and (d) an enzyme is further disclosed. The NAD(P) mimics are I [R = CN, CONH2, CONHMe, CSNH2, COCH3, COOMe; R1 = CH2(CH2O)nYR2, ribose-YR2, or (X substituted)benzyl; Y = OP(:O)O, OBO2, OSO2, NHMe, (CH2)nNH, adenine, imidazole; R2 = H, Me, (OCH2CH2)n, (NCH2CH2)n, [N:P(OMe)2]n; X = OMe, CF3, (OCH2CH2)n, OP(:O)OR3; R3 = H, Me, (OCH2CH2)n, (NCH2CH2)n, [N:P(OMe)2]n; n = 1-2000] and salts thereof. Thus, I with R1 = benzyl and R = various substituents such as CONH2 as well as I with R1 = ribose 5'-methylphosphate and R = CONH2 were synthesized and studied. Both of these coAlc. dehydrogenase enzyme mimics were used by horse liver alc. dehydrogenase to reduce phenethylmethylketone to the corresponding alc. with >93% ee (S-enantiomer). The reduced mimics were produced in this reaction using [Cp*Rh(bpy)(H2O)](OTf)2 as a catalyst precursor and sodium formate as hydride source.

ST pyridinium deriv NAD NADP mimic enzymic oxidn redn

IT 1445-91-6P 22148-86-3P 26184-62-3P 61277-90-5P 74709-08-3P 459165-24-3P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)

IT 9031-72-5, Alcohol dehydrogenase 9035-73-8, Oxidase 9037-80-3, Reductase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(NAD(P) mimic for use in enzymic redox reactions)

IT 100-44-7P, Benzyl chloride, biological studies 237417-60-6P 237417-65-1P 416846-01-0P 416846-02-1P 459165-14-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)

IT 388078-51-1P **459165-10-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)

IT 93-60-7 98-86-2, Phenylmethylketone, reactions 98-92-0, Nicotinamide 100-54-9, 3-Cyanopyridine 107-87-9, Methylethylketone 108-99-6, 3-Methylpyridine 350-03-8, 3-Acetyl pyridine 366-18-7, 2,2'-Bipyridyl 1007-32-5, Benzylethylketone 1094-61-7 2550-26-7, Phenethylmethylketone 2630-41-3 4621-66-3, Thionicotinamide 29583-35-5 53830-52-7, 3-Pyridinecarbothioamide, n-methyl- 70887-29-5, p-Methoxybenzyl iodide 165751-23-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(NAD(P) mimic for use in enzymic redox reactions)

IT 6456-44-6P 194208-27-0P 237417-62-8P 237417-63-9P 237417-66-2P 237417-67-3P 237417-68-4P 237417-69-5P 237426-33-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(NAD(P) mimic for use in enzymic redox reactions)

IT 53-59-8, NADP 53-84-9, NAD

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mimics; NAD(P) mimic for use in enzymic redox reactions)

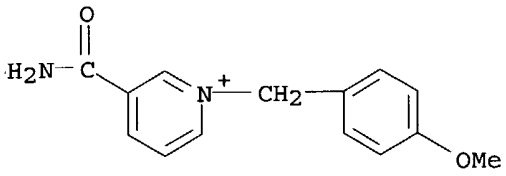
IT **459165-10-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)

RN 459165-10-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

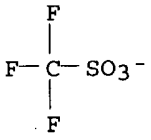
CM 1

CRN 175979-55-2
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S



L57 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:675770 HCAPLUS
DN 137:216955
ED Entered STN: 08 Sep 2002
TI Method for treating fibrotic diseases or other indications using thiadiazolium, pyridinium and pyrimidinium salts
IN Wagle, Dilip; Gall, Martin; Bell, Stanley C.; Lavoie, Edmond J.
PA Alteon, Inc., USA
SO PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002067851	A2	20020906	WO 2001-US49833	20011228
WO 2002067851	A3	20030206		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,

VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1355645 A2 20031029 EP 2001-273859 20011228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
US 2002183365 A1 20021205 US 2001-36857 20011231
US 2004097495 A1 20040520 US 2003-691839 20031023
PRAI US 2000-259294P P 20001229
US 2001-259238P P 20010102
US 2001-296246P P 20010606
WO 2001-US49833 W 20011228
US 2001-36857 A1 20011231
OS MARPAT 137:216955

AB The title compds. YAr+X- [I; Ar = 5-6 membered heteroaryl ring having a first ring N atom and optionally second or third ring N atoms, with the remaining ring atoms being C, O, or S, (provided the first N atom of Ar is a quaternary N and Ar is not thiazolium, oxazolium or imidazolium); Y is substituted on the first ring N atom (with the proviso that if Ar is pyrazole, indazole, triazole, benzotriazole, the second ring N atom is substituted with alkyl, alkoxycarbonylalkylene, aryl, etc.); Ar can be substituted on ring C atoms with aryl, carbamoyl, aralkyl, etc.; Y = CHR5R6 (R5 = H, alkyl, cycloalkyl, etc.; R6 = H, alkyl, alkenyl, etc.); X = a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt], useful in treating or ameliorating certain fibrotic diseases or other indications linked to or associated with the formation of excess collagen, in an animal, including a human, were prepared Thus, refluxing 2-aminothiadiazole with 2-bromoacetamide in MeCN for 5 h afforded 5-amino-3-carbamoylmethyl-[1,3,4]thiadiazolium bromide. Assays to determine the activity of compds. I in breaking, reversing or inhibiting the formation of advanced glycosylation end products (AGEs) or AGE-mediated cross-links was presented (no data).

ST thiadiazolium pyridinium pyrimidinium salt prepn advanced glycosylation endproduct AGE; fibrosis thiadiazolium pyridinium pyrimidinium salt prepn

IT Glycoproteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(AGE (advanced glycosylation end product); preparation of thiadiazolium, pyridinium and pyrimidinium salts for reversing advanced glycosylation cross-links)

IT Intestine, disease
(Crohn's, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Artery, disease
(arteritis, treatment of temporal; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Prostate gland, disease
(benign hyperplasia, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

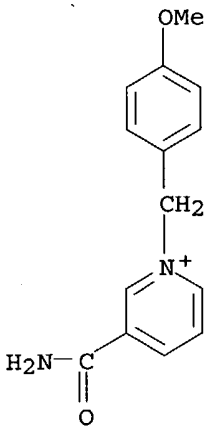
IT Mammary gland, disease
(fibrocystic, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Liver, disease
Lung, disease
Skin, disease
(fibrosis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Muscle, disease
(hypertrophy, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Intestine, disease
(inflammatory, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Connective tissue, disease
(mixed connective tissue disease, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Muscle, disease
(myositis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Artery, disease
(periarteritis nodosa, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Pleura, disease
(pleurisy, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Anti-inflammatory agents
Human
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Connective tissue, disease
(scleroderma, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Nervous system, disease
(sclerosis, treatment of cerebrosclerosis, annular sclerosis, diffuse sclerosis and lobar sclerosis; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Cystic fibrosis
Fibrosis
Hypertrophy
Sarcoidosis
(treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Blood vessel, disease
(vasculitis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT 13076-43-2P **63828-55-7P** 454704-85-9P 454704-86-0P
454704-87-1P 454704-88-2P 454704-89-3P 454704-90-6P 454704-91-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT 98-92-0, Nicotinamide 100-39-0, Benzyl bromide 104-83-6,
4-Chlorobenzyl chloride 289-95-2, Pyrimidine 456-04-2 459-46-1,
4-Fluorobenzyl bromide 589-17-3, 4-Bromobenzyl chloride 683-57-8,
2-Bromoacetamide 824-94-2, 4-Methoxybenzyl chloride 937-20-2,
2-Chloro-1-(4-chlorophenyl)ethanone 4005-51-0, 2-Aminothiadiazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT **63828-55-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L57 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:619241 HCAPLUS
DN 125:300276
ED Entered STN: 18 Oct 1996
TI Reactions of Charged Substrates. 5. The Solvolysis and Sodium Azide Substitution Reactions of Benzylpyridinium Ions in Deuterium Oxide
AU Buckley, Neil; Oppenheimer, Norman J.
CS Department of Pharmaceutical Chemistry, University of California, San Francisco, CA, 94143-0446, USA
SO Journal of Organic Chemistry (1996), 61(21), 7360-7372
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 7
AB Second-order rate consts. and activation values were measured for the reactions with NaN3 of a series of 4-Y-substituted (Y = MeO, Me, H, Cl, and NO2) benzyl 3'-Z-substituted (Z = CN, CONH2, H, F, Ac) pyridinium chlorides in deuterium oxide. 3'-Cyanopyridine substrates reacted much faster than nicotinamide and pyridine substrates; in the pyridine series the 4-Me, 4-H, and 4-Cl benzyl analogs did not react for up to 6 mo at 96° in 1.7 M NaN3. The 3'-cyanopyridine substrates do not exhibit borderline kinetic behavior, but the nicotinamide substrates do. The Hammett plot is flat for the NaN3 reaction of 3'-cyanopyridine substrates and increasingly V-shaped for the nicotinamide and pyridine substrates. The values of βLG (four-point plot) for the NaN3 reaction of the 4-MeO benzyl substrates is -1.45, which is usually interpreted as being a very "late" activated complex. Two-point Bronsted "plots" for the other benzyl derivs. and for two N-methylpyridinium ions give values of βLG in the same range. The second-order rate constant and activation values for N-methyl-3'-cyanopyridinium iodide are within the same range as those for the benzyl substrates. For the hydrolysis reaction, the Hammett plot is linear for 3'-cyanopyridine substrates (ρ+ = -1.24) and flat for the nicotinamide substrates. The extent of hydrolysis of 0.005-0.05 M solns. of the 3'-cyanopyridinie substrates depended on the initial concentration of substrate, and hydrolysis was slowed significantly or stopped completely in the presence of exogenous 3-cyanopyridine. These results show that an equilibrium is established among the products for the 4-MeO, 4-Me, 4-H, and

4-Cl substrates; the 4-NO2 substrate reacted too slowly to discern any difference. Data for the extent of hydrolysis were fitted by an equation derived assuming the equilibrium Despite this limitation on a classic test of mechanism, the rates and ρ values are consistent with direct displacement by solvent and not with a unimol. process. These results, which are rationalized in terms of the Pross-Shaik model, suggest that there are no ion-dipole complex intermediates in the benzyl series and show that borderline kinetic behavior is a function of leaving group ability and is not necessarily related to a change in mechanism. A computational approach was used to evaluate anomalous βLG values for the hydrolysis and nucleophilic substitution reactions of the methylpyridinium ion substrates. It was found that neither the Nu-substrate bond lengths nor the difference in charge matched the βLG values. The value of ΔΔS.thermod. of -15 gibbs/mol between (4-methoxybenzyl)-3'-cyanopyridinium chloride and the corresponding dimethylsulfonium chloride in the NaN3 reaction, which is the result of the solvation of the pyridine at the transition state and the lack of solvation of SMe2, is used to argue that the source of NAD+ glycohydrolase "catalysis" of NAD+ bond cleavage is the result of desolvation of the leaving group upon binding.

ST benzylpyridinium hydrolysis azide substitution kinetics mechanism; reaction const benzylpyridinium hydrolysis azide substitution; NAD glycohydrolase catalysis

IT Electron configuration and Electron density
Heat of hydrolysis
Hydrolysis
Kinetics of hydrolysis
Leaving group effects
Linear free energy relationship
Potential energy surface and hypersurface
Reaction constant
Substituent effect
Substitution reaction, nucleophilic
Transition state structure
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Pyridinium compounds
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Molecular orbital
(frontier, kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Heat of substitution reaction
Kinetics of substitution reaction
(nucleophilic, kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT 2876-13-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(estimated; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

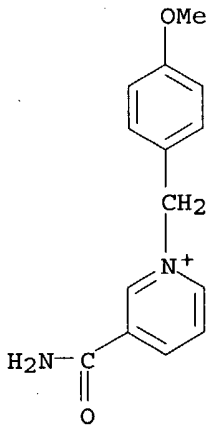
IT 594-09-2, Trimethylphosphine 1004-16-6, 3-Cyano-1-methylpyridinium iodide 4329-72-0 5096-13-9 6456-44-6 6621-73-4 6951-52-6 14343-69-2, Azide 14535-08-1 14535-12-7 20461-54-5, Iodide, reactions 26628-22-8, Sodium azide 52354-19-5 **63828-55-7** 74796-72-8 76053-06-0 87976-56-5 98349-72-5 183054-49-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT 7732-18-5, Water, reactions 15923-33-8 183054-50-4

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(potential surface calcn.; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT **63828-55-7**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L57 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:191937 HCAPLUS
DN 124:316412
ED Entered STN: 04 Apr 1996
TI Reactions of Charged Substrates. 4. The Gas-Phase Dissociation of (4-Substituted benzyl)dimethylsulfoniums and -pyridiniums
AU Buckley, Neil; Maltby, David; Burlingame, Alma L.; Oppenheimer, Norman J.
CS School of Pharmacy, University of California, San Francisco, CA, 94143-0446, USA
SO Journal of Organic Chemistry (1996), 61(8), 2753-62
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-12 (Physical Organic Chemistry)
Section cross-reference(s): 33
AB The relative rates for the gas-phase dissociation RX+ → R+ + X° of five (4-Y-substituted benzyl)dimethysulfoniums (Y = MeO, Me, H, Cl, and NO2) and 24 (4-Y-substituted benzyl)-3'-Z-pyridiniums (complete series for Z = CN, Cl, CONH2, and H, and 4-methoxy- and 4-nitrobenzyls for Z = F and CH3CO) were measured using liquid secondary ion mass spectrometry. The Hammett plot (vs δΔG0 or σ+) is linear for the sulfoniums, but plots for the four pyridinium series have a drastic break between the 4-Cl and 4-NO2 substrates. Broensted-like plots for the pyridiniums show a strong leaving group effect only for 4-nitrobenzyls. An anal. of these linear free energy relations with supporting evidence

from semiempirical computations suggests that collisionally activated pyridinium substrates dissociate through two pathways, direct dissociation and an ion-neutral complex intermediate. Comparison of these results with results for the solution reactions of some of these compds. shows that the mechanism is different in the gas and solution phases. Sufficient exptl. data are not available to assign a mechanism for dissociation to the sulfonium series, but computational results show characteristics of a direct dissociative mechanism.

ST dissocn gas phase benzyldimethylsulfonium benzyldimethylpyridinium; sulfonium benzyldimethyl gas phase dissocn; pyridinium benzyldimethyl gas phase dissocn

IT Linear free energy relationship
Reaction constant
(for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT Dissociation
Kinetics of dissociation
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT Leaving group effects
Substituent effect
(on gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

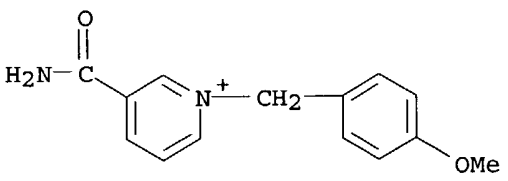
IT Linear free energy relationship
(Broensted, for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT 15519-25-2 16183-83-8 16183-87-2 24837-70-5 38332-27-3
45809-04-9 45964-81-6 46122-80-9 46441-13-8 48120-95-2
58219-38-8 58219-39-9 71897-24-0 71897-27-3 78186-22-8
133227-04-0 **175979-55-2** 175979-56-3 175979-57-4
175979-58-5 175979-59-6 175979-60-9 175979-61-0 175979-62-1
175979-63-2 175979-64-3 175979-65-4 175979-66-5 175979-67-6
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT **175979-55-2**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

RN 175979-55-2 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L57 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:422794 HCAPLUS

DN 113:22794

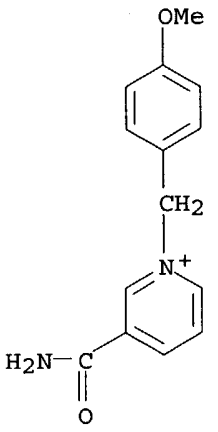
ED Entered STN: 21 Jul 1990

TI Addition of cyanide ion to nicotinamide cations in acetonitrile. Formation of nonproductive charge-transfer complexes

AU Engbersen, Johan F. J.; Koudijs, Arie; Sleiderink, Hedwig M.; Franssen,

Maurice C. R.
CS Lab. Org. Chem., Agric. Univ., Wageningen, 6703 HB, Neth.
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1990), (1), 79-83
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
OS CASREACT 113:22794
AB The mixing of equal vols. of 0.2 mmol dm-3 1-benzylnicotinamide ion and 2 mmol dm-3 cyanide ion results in the immediate formation of a transient absorption band at 375 nm which can be ascribed to a charge-transfer complex. This complex disappears within ca. 0.2 s with the formation of the 1,6-addition product which, in turn, is rapidly converted into the thermodynamically more stable 1,4-adduct. Me substitution at the 6-position of the nicotinamide ring inhibits the formation of the 1,6-adduct, resulting in an increase in the lifetime of the charge-transfer complex. Subsequently a mixture of the 1,4-cyanide adduct and, most likely, the 1,2-adduct is formed. Rate effects with variation of substituents in the 1-benzyl group reveal that charge-transfer complex formation is counterproductive to the formation of addition products.
ST cyanide ion addn nicotinamide cation; charge transfer complex cyanide nicotinamide; substituent effect cyanide addn nicotinamide
IT Reaction constant
(for addition, dissociation, and charge-transfer-complexation processes in cyanide ion-nicotinamide cation systems)
IT Addition reaction
(of cyanide ion with nicotinamide cations, formation of nonproductive charge-transfer complexes in)
IT Kinetics of addition reaction
(of cyanide ion with nicotinamide cations, solvent and substituent effects on)
IT Kinetics of dissociation
(of cyanide-ion adducts with nicotinamide cations, solvent and substituent effects on)
IT Ultraviolet and visible spectra
(of transient species, in addition reaction of cyanide ion with nicotinamide cations)
IT Substituent effect
(on addition, dissociation, and charge-transfer-complexation processes in cyanide ion-nicotinamide cation systems)
IT 151-50-8, Potassium cyanide (K(CN))
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with nicotinamide cations)
IT 127678-22-2 127678-24-4 127678-25-5 127678-27-7 127678-29-9
RL: PROC (Process)
(decay of, kinetics of)
IT 13076-43-2P 54027-58-6P 63761-90-0P 63761-95-5P **63828-55-7P**
70293-11-7P 127663-01-8P 127663-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with cyanide)
IT 96551-72-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation and addition reaction of, with cyanide)
IT 127663-05-2P 127663-06-3P 127663-07-4P 127678-20-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation of, with cyanide)
IT 19432-61-2P 75420-69-8P 75420-70-1P 75420-71-2P 75420-74-5P
127663-03-0P 127663-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation of, kinetics of)

IT 127663-08-5P 127663-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with cyanide)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L57 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:166806 HCAPLUS
DN 108:166806
ED Entered STN: 13 May 1988
TI Polarographic reduction of p-substituted 1-phenyl-3-(aminocarbonyl)pyridinium salts
AU Krechl, Jiri; Mizaninoiva, Daniela; Volke, Jiri; Kuthan, Josef
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28, Czech.
SO Collection of Czechoslovak Chemical Communications (1987), 52(6), 1550-60
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 72
AB The substituent effect (H, NO2, CO2H, Br, Cl, NHAc, Me, OMe, OH, NEt2) on the polarog. behavior of p-substituted 1-phenyl-3-aminocarbonylpyridinium cations has been investigated, in particular on their half-wave potentials in aqueous phosphate buffers pH 6·65 (10% DMF) and in anhydrous solns. of DMF with 0·05 mol L-1 Bu4N+ BF4- as supporting electrolyte. The half-wave potentials of the reduction wave which corresponds to the uptake of a single electron (wave B) and to the formation of the primary radical, obey a Hammett correlation in a way similar to the case of 1-benzyl-3-aminocarbonylpyridinium cations. The slope Qπ,R in the Hammett plot equals 0·093 V for 10% DMF and 0·179 V for anhydrous DMF and compares thus with the slope obtained with the 1-benzyl derivs. where 0.05 V was found for water and 0·127 V of anhydrous acetonitrile. The transfer of the substituent effect from the substituent in the para position on the benzene nucleus to the heterocyclic ring is

thus equally active in both substances and depends more strongly on the solvent than on the structure of the cation of both types. The low sensitivity in both series towards a change in the substituent is explained by the fact that during the uptake of the electron the benzene and the pyridine nucleus are not even approx. coplanar. This is why the π-overlap between the two nuclei is considerably restricted. The anal. of sampled d.c.-polarog. waves has confirmed that the one-electron uptake is followed by a chemical reaction, most probably a dimer formation or a reaction of the primary product with the starting substance.

ST polarog redn pyridinium salt; amidopyridinium phenyl electrochem redn LFER

IT Reduction
(of substituted phenyl(aminocarbonyl)pyridinium salts, substituent effects on)

IT Substituent effect
(on polarog. reduction of phenyl(aminocarbonyl)pyridinium salts)

IT 5096-13-9 6951-52-6 52354-19-5 **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)

IT 54027-59-7P 54027-60-0P 69986-64-7P 76911-53-0P 76911-55-2P 76911-56-3P 87384-49-4P 87384-51-8P 87384-52-9P 112445-86-0P 113849-47-1P 113849-48-2P 113849-49-3P 113849-50-6P 113849-53-9P 113849-54-0P 113849-55-1P 113849-57-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and polarog. reduction of)

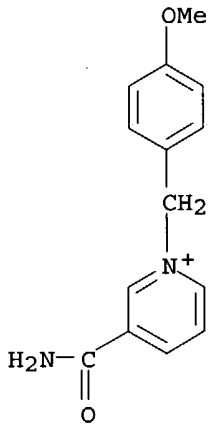
IT 98-92-0, Nicotinamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with anilines)

IT 62-53-3, reactions 93-05-0 100-01-6, reactions 104-94-9, 4-Methoxyaniline 106-40-1, 4-Bromoaniline 106-47-8, 4-Chloroaniline, reactions 106-49-0, reactions 122-80-5, 4-Acetamidoaniline 123-30-8, 4-Hydroxyaniline 150-13-0, 4-Aminobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nicotinamide)

IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)

RN 63828-55-7 HCAPLUS

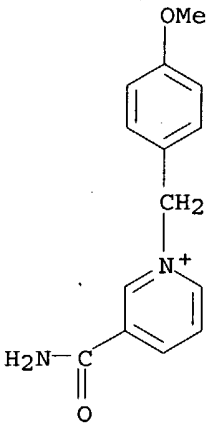
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



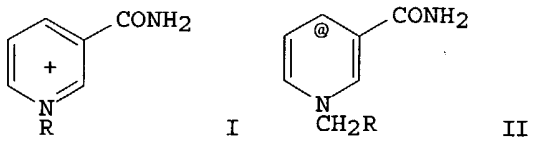
● Cl⁻

L57 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:422428 HCAPLUS
DN 103:22428
ED Entered STN: 27 Jul 1985
TI Selective reduction of pyridinium, quinolinium, and pyrazinium salts to the dihydro stage with 1-benzyl-1,2-dihydroisonicotinamide
AU Nuvole, Antonio; Paglietti, Giuseppe; Sanna, Paolo; Acheson, R. Morrin
CS Ist. Chim. Farm., Univ. Sassari, Sassari, 07100, Italy
SO Journal of Chemical Research, Synopses (1984), (11), 356-7
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 22, 28
OS CASREACT 103:22428
AB Quinolinium, pyridinium, and pyrazinium salts were reduced selectively to 1,4-dihydroquinolines, 1,4-dihydropyridines, and 1,6-dihydropyrazines, resp., by 1-benzyl-1,2-dihydroisonicotinamide (I) in dry MeOH under N. E.g., reduction of N-benzyl-3-carbamoylquinolinium bromide by I for 5 min gave N-benzyl-1,4-dihydroquinoline-3-carboxamide quant.
ST benzylisonicotinamide redn quinolinium pyridinium pyrazolinium; isonicotinamide benzyl redn quaternary compd; regioselective redn quaternary compd benzylisonicotinamide; quinolinium redn benzylisonicotinamide regioselective; pyridinium redn benzylisonicotinamide regioselective; pyrazinium redn benzylisonicotinamide regioselective
IT Regiochemistry
(of reduction of quinolinium, pyridinium, or pyrazinium compds. by benzyldihydroisonicotinamide)
IT Reduction
(regioselective, of quinolinium, pyridinium, and pyrazinium compds. by benzyldihydroisonicotinamide)
IT 62417-98-5P 96421-80-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and selective reduction of, by benzyldihydroisonicotinamide)
IT 96421-81-7P 96421-82-8P 96421-83-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 952-92-1P 2288-38-2P 17260-79-6P 17750-23-1P 19350-64-2P
20224-92-4P 34865-02-6P 37589-77-8P 56133-30-3P 57355-62-1P
71127-33-8P 73027-91-5P 74124-15-5P 78224-91-6P 88928-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by selective reduction of quaternary compound with benzyldihydroisonicotinamide)
IT 100-39-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization by, of Me quinolinecarboxylate, cyanopyridine, and pyrazinecarboxamide)
IT 98-96-4 100-48-1 53951-84-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of, by benzyl bromide)
IT 75532-98-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by, of quinolinium, pyridinium, and pyrazinium compds., regioselective)
IT 5496-66-2 6456-44-6 6516-41-2 6516-53-6 13076-43-2 13958-90-2
26368-94-5 **63828-55-7** 70293-11-7 73027-90-4 96421-79-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by benzyldihydroisonicotinamide, regioselective)
IT **63828-55-7**

RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by benzyldihydroisonicotinamide, regioselective)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



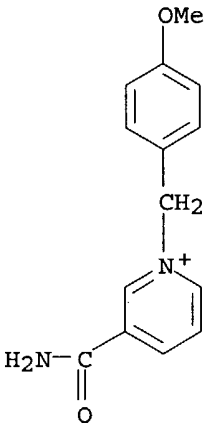
L57 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:504507 HCAPLUS
DN 99:104507
ED Entered STN: 12 May 1984
TI Dihydropyridines. XLVIII. Substituent effect in addition of cyanide ion to p-substituted 1-benzyl-3-carbamoylpyridinium chlorides
AU Pavlikova-Raclova, Frantiska; Kuthan, Josef
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (1983), 48(5), 1401-7
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
GI



AB Rate consts. for the title reaction were determined in aqueous solns. of 8 quaternary salts of nicotinamide (I; R = p-XC6H4CH2; X = MeO, Me, H, F,Cl, CO2Me, cyano, NO2). Good Hammett correlations were found, along with correlation of E1/2 of polarog. reduction of I with rate and equilibrium consts.

In aqueous media, reduction of I (same R; X = Me, H, F, Cl, MeO) with π-donor substituents proceeds via a simple E mechanism I → II, whereas in the case of π-acceptor substituents (I; X = NO2, CN, CO2Me), radicals II are formed via a 3-step CEC mechanism.

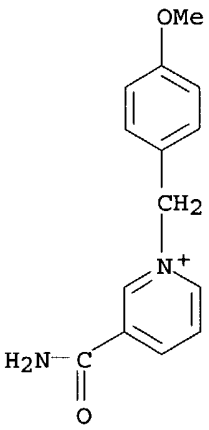
ST cyanation benzylcarbamoylpyridinium kinetics mechanism; LFER cyanation benzylcarboamoylpyridinium
IT Linear free energy relationship
(in cyanation of benzylcarbomoylpyridinium chlorides)
IT Cyanation
(of benzylcarbamoylpyridinium chlorides, mechanism of)
IT Kinetics of cyanation
Reduction, electrochemical
(of benzylcarbomoylpyridinium chlorides)
IT 1652-58-0 5096-13-9 6621-73-4 6951-52-6 52354-19-5
63828-55-7 84354-35-8 84389-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L57 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:61940 HCAPLUS
DN 98:61940
ED Entered STN: 12 May 1984
TI Polarographic reduction of p-substituted 1-benzyl-3-carbamoylpyridinium chlorides
AU Kuthan, Josef; Pavlikova-Raclova, Frantiska
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (1982), 47(11), 2890-903
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 72-2 (Electrochemistry)
AB Substituent effects (H, NO2, CN, CO2Me, Me, MeO, Me2N, Cl, F) on polarog. characteristics of the title quaternary salts were studied in H2O, anhydrous MeCN, and aqueous EtOH. In the last solvent, 1 of the polarog. waves gradually disappears. The probable course of the investigated electrode processes and accompanying chemical transformations is discussed.

ST polarog redn benzyl carbamoylpyridinium chloride; quaternary nicotinamide chloride polarog redn
IT Substituent effect
(in polarog. reduction of benzylcarbamoylpyridinium chlorides)
IT Reduction, electrochemical
(of benzylcarbamoylpyridinium chloride p-substituted derivs.)
IT 1652-58-0 5096-13-9 6621-73-4 6951-52-6 52354-19-5
63828-55-7 84354-35-8 84389-20-8 84389-21-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)
IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L57 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:480366 HCAPLUS
DN 87:80366
ED Entered STN: 12 May 1984
TI Model dehydrogenase reactions. Catalysis of dihydronicotinamide reductions by noncovalent interactions
AU Hajdu, Joseph; Sigman, David S.
CS Sch. Med., Univ. California, Los Angeles, CA, USA
SO Biochemistry (1977), 16(13), 2841-6
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
CC 7-4 (Enzymes)
AB Carboxylate, pyrophosphate, and hydroxyl groups can accelerate the nonenzymic rates of dihydronicotinamide redns. via intramol. noncovalent interactions. The accelerations by the neg. charged carboxylate and pyrophosphate groups occur in nonpolar solvents but the effect of the hydroxyl groups occurs both in aqueous and nonaq. solution The largest effects are observed for neighboring carboxylate groups in nonpolar solvents; e.g., the 2nd-order rate constant for the reduction of N-methylacridinium ion by N-cis-2'-carboxycyclopentyldihydronicotinamide in acetonitrile is 1000-fold more rapid than the rate constant for the corresponding Me ester.

Apparently, the neg. charged carboxylate stabilizes the partial pos. charge which develops on the nicotinamide moiety in the transition state. The conclusion that the neg. charged pyrophosphate can enhance dihydronicotinamide redns. is based on the observation that β-NADH reduces N-methylacridinium ion 30-fold faster in MeOH than in aqueous solution, whereas α-NADH reduces the oxidant only 7-fold faster in MeOH than in water. The pyrophosphate group enhances the reaction rates of both anomers by a distance-dependent field effect. The magnitude is greater for the β anomer because the pyrophosphate and nicotinamide moieties are nearer neighbors in this anomer. The rate accelerations produced by hydroxyl groups of alcs. are not as great as those observed for carboxylate groups in nonpolar solvents. In aqueous solns., α-NADH reduces 3 different oxidants 10-fold more rapidly than β-NADH. In acetonitrile, synthetic dihydronicotinamides containing hydroxyl groups increase the rate 6-fold. These modest accelerations with the neutral hydroxyl groups emphasize the importance of a neg. charged group in order to achieve large enhancements in nonaq. solns.

ST dehydrogenase model dihydronicotinamide redn

IT Functional groups
(diphosphate, in dihydronicotinamide reduction of methylacridinium, dehydrogenase reaction mechanism in relation to)

IT Carboxyl group
Hydroxyl group
(in dihydronicotinamide reduction of methylacridinium, dehydrogenase reaction mechanism in relation to)

IT Kinetics of reduction
(of methylacridinium, by alkyldihydronicotinamide derivs.)

IT 58-68-4D, analogs 21104-13-2 56133-27-8 56133-28-9 56133-30-3
56133-31-4 56133-32-5 56133-33-6 63761-81-9 63761-82-0
63761-83-1 63761-84-2 63761-85-3 63761-86-4 63761-87-5
63761-88-6 63762-01-6 63762-02-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-methylacridinium reduction by, dehydrogenase reaction mechanism in relation to)

IT 17750-24-2
RL: PRP (Properties)
(UV spectra of, solvent effect on)

IT 63762-03-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(chloranil reduction by, dehydrogenase reaction mechanism in relation to)

IT 9035-82-9
RL: PRP (Properties)
(models for, N-alkyldihydronicotinamide as)

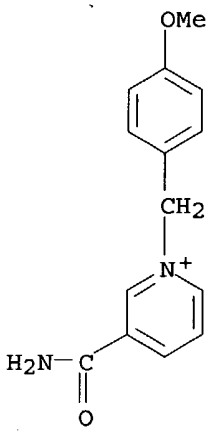
IT 5096-13-9P 7597-54-8P 63761-89-7P 63761-90-0P 63761-91-1P
63761-92-2P 63761-93-3P 63761-94-4P 63761-95-5P 63761-96-6P
63761-97-7P 63761-98-8P 63761-99-9P 63762-00-5P **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

IT 118-75-2, reactions 13367-81-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by dihydronicotinamide alkyl derivs., dehydrogenase reaction mechanism in relation to)

IT **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L57 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1963:454780 HCAPLUS
DN 59:54780
OREF 59:**9970a-c**
ED Entered STN: 22 Apr 2001
TI Action of base on quaternary salts of nicotinamide
AU Dittmer, Donald C.; Kolyer, J. M.
CS Univ. of Pennsylvania, Philadelphia
SO Journal of Organic Chemistry (1963), 28(9), 2288-94
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
CC 37 (Heterocyclic Compounds (One Hetero Atom))
GI For diagram(s), see printed CA Issue.
AB Treatment of 1benzyl-3-carbamoylpyridinium chloride with NaOH in dilute EtOH yielded a new' substance (I), believed to be a cyclic trimer. The structure of I was based on its analysis, infrared spectrum, ultraviolet spectrum, fluorescence spectrum, proton magnetic resonance spectrum, mol. weight, and its chemical reactions. I is believed to have been formed by way of
a pyridinium ylide. Several new pseudo base ethers of 1-substituted nicotinamide salts have been prepared
IT Spectra, visible and ultraviolet
(of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]-heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
IT Spectra, infrared
(of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
IT Nuclear magnetic resonance
(of 1,6,11-triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
IT Bases
(reactions of, with 3-carbamoylpyridinium derivs.)
IT Nitrone, α-benzyl-N-[p-(dimethylamino)phenyl]-α-phenyl-
Pyridinium, 1-(p-bromobenzyl)-3-carbamoyl-, chloride
Pyridinium, 1-benzyl-3-carbamoyl-, oxalate
Pyridinium, 1-benzyl-3-carbamoyl-, picrate
Pyridinium, 3-carbamoyl-1-(2,4-dinitrobenzyl)-, chloride
Pyridinium, 3-carbamoyl-1-(p-methoxybenzyl)-, chloride

Pyridinium, 3-carbamoyl-1-(p-nitrobenzyl)-, chloride
IT Pyridinium, 3-carbamoyl-
(derivs., reaction with bases)
IT 952-92-1, Nicotinamide, 1-benzyl-1,4-dihydro- 1652-58-0, Pyridinium, 3-carbamoyl-1-(p-fluorobenzyl)-, chloride 1893-57-8, Nicotinamide, 1-(p-fluorobenzyl)-1,4-dihydro- 2996-08-9, Nicotinamide, 4,4'-oxybis[1-(p-fluorobenzyl)-1,4-dihydro- 4533-64-6, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-fluorophenyl)- 5096-13-9, Pyridinium, 1-benzyl-3-carbamoyl-, chloride 6951-52-6, Pyridinium, 3-carbamoyl-1-(p-chlorobenzyl)-, chloride 13502-54-0, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,4-dihydro- 19355-18-1, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,6-dihydro- 75340-29-3, Nicotinamide, 4,4'-oxybis[1-benzyl-1,4-dihydro- 92578-90-0, Glycine, N-(p-tolylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93807-08-0, Glycine, N-(phenylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93946-35-1, Glycine, N-(p-tolylsulfonyl)-, 2-(m-bromophenyl)hydrazide 94379-06-3, Nipecotamide, 1-benzyl-, picrate 95945-13-4, Nicotinamide, 4,4'-oxybis[1,4-dihydro-1-(p-nitrobenzyl)- 96003-72-4, Nicotinamide, 4,4'-oxybis[1-(2,6-dichlorobenzyl)-1,4-dihydro- 96635-71-1, Nipecotamide, 1-benzyl-, hydrochloride 106141-61-1, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-bromophenyl)- 106141-62-2, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-chlorophenyl)- 106141-68-8, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-triphenyl-
(preparation of)

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FILE 'USPATFULL' ENTERED AT 16:11:32 ON 23 JUN 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 16:11:32 ON 23 JUN 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr tot l56

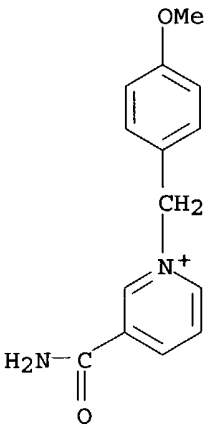
L56 ANSWER 1 OF 4 USPATFULL on STN
AN 2004:127511 USPATFULL
TI Method for treating fibrotic diseases or other indications IIIC
IN Wagle, Dilip, New York, NY, UNITED STATES
Gall, Martin, Morristown, NJ, UNITED STATES
Bell, Stanley C., Narberth, PA, UNITED STATES
LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES
PI US 2004097495 A1 20040520
AI US 2003-691839 A1 20031023 (10)
RLI Continuation of Ser. No. US 2001-36857, filed on 31 Dec 2001, PENDING
PRAI US 2000-259294P 20001229 (60)
US 2001-259238P 20010102 (60)
US 2001-296246P 20010606 (60)
DT Utility
FS APPLICATION
LREP MINTZ, LEVIN, COHN, FERRIS, GLOVSKY, AND POPEO, P.C., ONE FINANCIAL CENTER, BOSTON, MA, 02111
CLMN Number of Claims: 49
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 3287
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided is a method of treating or ameliorating certain fibrotic diseases or other indications in an animal, including a human,

comprising administering an effective amount of a compound of the formula I:

Y--Ar.sup..sym..X.sup.-

wherein Ar.sup..sym. is heteroaryl with a quaternary nitrogen, Y defines certain substitutions on the quaternary nitrogen, and X.sup.- is anion.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **63828-55-7P**
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
RN 63828-55-7 USPATFULL
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

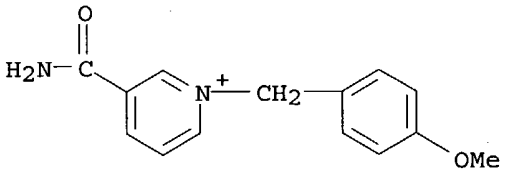
L56 ANSWER 2 OF 4 USPATFULL on STN
AN 2003:30319 USPATFULL
TI Novel agents for replacement of NAD+/NADH system in enzymatic reactions
IN Fish, Richard H., Berkeley, CA, UNITED STATES
Kerr, John B., Oakland, CA, UNITED STATES
Lo, Christine H., Solana Beach, CA, UNITED STATES
PI US 2003022266 A1 20030130
US 6716596 B2 20040406
AI US 2001-805726 A1 20010312 (9)
DT Utility
FS APPLICATION
LREP Hana Verny, Peters, Verny, Jones & Biksa LLP, 385 Sherman Avenue, Suite 6, Palo Alto, CA, 94306
CLMN Number of Claims: 18
ECL Exemplary Claim: 1
DRWN 8 Drawing Page(s)
LN.CNT 1777
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel agents acting as co-factors for replacement of NAD(P).sup.+/NAD(P)H co-enzyme systems in enzymatic oxido-reductive reactions. Agents mimicking the action of NAD(P).sup.+/NAD(P)H system in enzymatic oxidation/reduction of substrates into reduced or oxidized products. A method for selection and preparation of the mimicking agents

for replacement of NAD(P).sup.+/NAD(P)H system and a device comprising co-factors for replacement of NAD(P).sup.+/NAD(P)H system.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **459165-10-7P**
(NAD(P) mimic for use in enzymic redox reactions)
RN 459165-10-7 USPATFULL
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

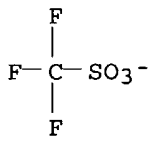
CM 1

CRN 175979-55-2
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S



L56 ANSWER 3 OF 4 USPATFULL on STN
AN 2002:323196 USPATFULL
TI Method for treating fibrotic diseases or other indications IIIC
IN Wagle, Dilip, New York, NY, UNITED STATES
Gall, Martin, Morristown, NJ, UNITED STATES
Bell, Stanley C., Narberth, PA, UNITED STATES
LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES
PI US 2002183365 A1 20021205
AI US 2001-36857 A1 20011231 (10)
PRAI US 2001-296246P 20010606 (60)
US 2001-259238P 20010102 (60)
US 2000-259294P 20001229 (60)
DT Utility
FS APPLICATION
LREP ALLEN BLOOM, C/O DECHERT, PRINCETON PIKE CORPORATION CENTER, P.O. BOX 5218, PRINCETON, NJ, 08543-5218
CLMN Number of Claims: 49
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 3334
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided is a method of treating or ameliorating certain fibrotic diseases or other indications in an animal, including a human, comprising administering an effective amount of a compound of the

formula I:

Y--Ar.sym..multidot.X.sup.--

wherein:

a. Ar is a five or six membered heteroaryl ring having a first ring nitrogen and optionally second or third ring nitrogens, with the remaining ring atoms being carbon, oxygen, or sulfur, provided the first nitrogen of Ar is a quaternary nitrogen and Ar is not thiazolium, oxazolium or imidazolium;

b. Y is substituted on the first ring nitrogen, with the proviso that if Ar is pyrazole, indazole, (1,2,3)-triazole, benzotriazole, or (1,2,4)-triazole, the second ring nitrogen is substituted

C. Y is:

1. a group of the formula --CH(R.sup.5)--R.sup.6 [as preferred in one embodiment]

(a) wherein R.sup.5 is hydrogen, alkyl, cycloalkyl-, alkenyl-, alkynyl-, aminoalkyl-, hydroxy[C.sub.1 to C.sub.6]alkyl, dialkylaminoalkyl-, (N-[C.sub.6 or C.sub.10]aryl)(N-alkyl)aminoalkyl-, piperidin-1-ylalkyl-, pyrrolidin-1-ylalkyl, azetidinylalkyl, 4-alkylpiperazin-1-ylalkyl, 4-alkylpiperidin-1-ylalkyl, 4-[C.sub.6 or C.sub.10]arylpiperazin-1-ylalkyl, 4-[C.sub.6 or C.sub.10]arylpiperidin-1-ylalkyl, azetidin-1-ylalkyl, morpholin-4-ylallcyl, thiomorpholin-4-ylalkyl, piperazin-1-ylalkyl, piperidin-1-ylalkyl, [C.sub.6 or C.sub.10]aryl, or independently the same as R.sup.6;

(b) wherein R.sup.6 is

(1) hydrogen, alkyl (which may be substituted by alkoxycarbonyl)-, alkenyl, alkynyl, cyano-, cyanoalkyl-, or Rs, wherein Rs is a [C.sub.6 or C.sub.10]aryl or a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms selected from the group consisting of oxygen, nitrogen and sulfur; or

(2) a group of the formula --W--R.sup.7 [as preferred in one embodiment], wherein R.sup.7 is alkyl, alkoxy, hydroxy, or Rs [as preferred in one embodiment], wherein W is --C(.dbd.O)-- or --S(O).sub.2--;

(3) a group of the formula --W--OR.sup.8 wherein R.sup.8 is hydrogen or alkyl,

(4) a group of the formula --CH(OH)Rs; or

(5) a group of the formula --W--N(R.sup.9)R.sup.10, wherein

(a) R.sup.9 is hydrogen and R.sup.10 is an alkyl or cycloalkyl, optionally substituted; or

(b) R.sup.9 is hydrogen or alkyl and R.sup.10 is Ar; or

(c) R.sup.9 is hydrogen or alkyl, R.sup.10 is a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms are selected from the group consisting of oxygen, nitrogen and sulfur; or

(d) R.sup.9 and R.sup.10 are both alkyl groups; or

(e) R.sup.9 and R.sup.10 together with N form a heterocycle containing

4-10 ring atoms which can incorporate up to one additional heteroatom selected from the group of N, O or S in the ring, wherein the heterocycle is optionally substituted; or

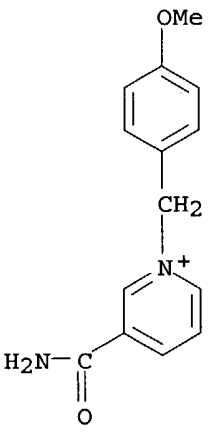
(f) R.sup.9 and R.sup.10 are both hydrogen; or

2. --NH.sub.2, and

e. X is a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt, or

(B) a pharmaceutically acceptable salt of the compound.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **63828-55-7P**
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
RN 63828-55-7 USPATFULL
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L56 ANSWER 4 OF 4 USPAT2 on STN
AN 2003:30319 USPAT2
TI Agents for replacement of NAD+/NADH system in enzymatic reactions
IN Fish, Richard H., Berkeley, CA, United States
Kerr, John B., Oakland, CA, United States
Lo, Christine H., Solana Beach, CA, United States
PA The Regents of the University of California, Oakland, CA, United States (U.S. corporation)
PI US 6716596 B2 20040406
AI US 2001-805726 20010312 (9)
DT Utility
FS GRANTED
EXNAM Primary Examiner: Gitomer, Ralph
LREP Verny, Hana
CLMN Number of Claims: 18
ECL Exemplary Claim: 1
DRWN 12 Drawing Figure(s); 7 Drawing Page(s)
LN.CNT 1759

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel agents acting as co-factors for replacement of NAD(P).sup.+/NAD(P)H co-enzyme systems in enzymatic oxido-reductive reactions. Agents mimicking the action of NAD(P).sup.+/NAD(P)H system in enzymatic oxidation/reduction of substrates into reduced or oxidized products. A method for selection and preparation of the mimicking agents for replacement of NAD(P).sup.+/NAD(P)H system and a device comprising co-factors for replacement of NAD(P).sup.+/NAD(P)H system.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

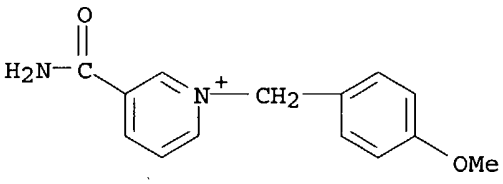
IT **459165-10-7P**
(NAD(P) mimic for use in enzymic redox reactions)

RN 459165-10-7 USPAT2

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

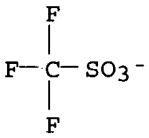
CM 1

CRN 175979-55-2
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S



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